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Free vibration of the water-filled single-walled carbon nanotubes

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Abstract

A double shell-potential flow model is developed to study the free vibration of the water-filled single-walled carbon nanotubes (SWCNTs) in the paper. SWCNTs are coupled with inner water via the van der Waals (vdW) interaction. It is shown that the vdW forces upshift the frequency of the SWCNTs. The results also reveal that the internal moving fluid plays an important role in the instability of system whereas the fluid velocity has very little influence on the dynamic characteristics of the tube.

Keywords: Water-filled single-walled carbon nanotubes; Free vibration; Van der Waals interaction

1. Introduction

The interaction of fluid with carbon nanotubes (CNTs) has become an attractive research topic in recent years, so a finer understanding of the dynamical behaviors of CNT-water system is essential to the development of the CNT-based nanodevices.

Up till now, considerable effort has been made to explore the vibration behavior of water-filled CNTs. For instance, Yan et al. [1, 2] and Wang et al. [3] as well as Khosravian et al. [4] discussed the dynamical stability behaviors of water-conveyed CNTs, and found that instability of the CNTs occurs at a critical flow velocity. However, there is little systematic consideration concerning the density of water in CNTs in these literature, and the overall density is usually fixed to the typical value $1g/cm^3$. Water molecules, in

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Fact, show at least two different ways in CNTs called "single-file mode" and "layered mode"[5].

Nomenclature

x	axial coordinate along tube length direction	t	time
R_t	radius	w_t	radial displacement,
E	Young's modulus	h	tube thickness,
D	flexural rigidity	ρ_t	mass density per unit area,
L	length	ρ_f	mass density per unit area,
R_f	radius	w_f	radial displacement,
γ	CNT–water surface tension	ρ_{water}	mass density per unit bulk
p	radial pressure	c	vdW interaction coefficient
$-0.6K$	well depth	s	interlayer spacing
s_0	equilibrium distance	$[I]$	identity matrix,
λ	eigenvalue	F	stress function F

Longhurt and Quirke [6] used layered mode to study the radial breathing vibration for single-walled CNTs (SWCNTs) with absorbed water. They considered the adsorbed fluid as an infinitesimally thin shell, which interacts with the nanotube via a continuum Lennard-Jones potential. Then, Wang et al. [7] developed a double shell-Stokes flow model to study the axisymmetric vibration of SWCNTs immerged in water. They modelled water in double layers- the absorbed layer of water molecules by SWCNTs and the water layer surrounding the absorbed layer. The approach greatly reduces the time required to simulate the interaction of absorbed water and CNTs and offers a theoretical explanation for the experimental observation and molecular dynamics simulations available in particular cases.

Motivated by these studies, for the first time, we develop a double shell- potential flow model to study the free vibration of the water-filled SWCNTs. Based on the model, discusses in detail will be shown below.

2. The double shell-potential flow model

The SWCNT-water system comprises three constituent parts, i.e., the SWCNTs, the absorbed layer of water molecules [6] and the water flow in the center of the SWCNTs. The SWCNTs and the internally absorbed layer of water are modeled as two-layer thin shells coupled via the interlayer vdW forces, and the water in the center of the SWCNTs is considered as the potential flow. By using the shell theory, the governing equations of the system are stated as

$$D\nabla^4 w_t + \rho_t \frac{\partial^2 w_t}{\partial t^2} = -c\left(w_t - w_f\right) + \frac{1}{R_t}\frac{\partial^2 F}{\partial x^2} \tag{1}$$

$$\gamma \frac{\partial^2 w_f}{\partial x^2} + \frac{R_t}{R_f} c\left(w_t - w_f\right) - p = \rho_f \frac{\partial^2 w_f}{\partial t^2} \tag{2}$$

$$\nabla^4 F = -\frac{Eh}{R_t}\frac{\partial^2 w_t}{\partial x^2} \tag{3}$$

$$p = \rho_{water}\frac{L}{m\pi}\frac{I_n\left(m\pi R_f / L\right)}{I_n'\left(m\pi R_f / L\right)}\left(\frac{\partial}{\partial t} + U\frac{\partial}{\partial x}\right)^2 w_f \tag{4}$$

where x is the axial coordinate along the tube length direction, t the time, $\nabla^4 = \left[\frac{\partial^2}{\partial x^2} + \frac{1}{R_i^2}\frac{\partial^2}{\partial \theta^2}\right]^2$ a differential operator, I_n the modified Bessel function of order n, prime($.'$) the derivative with respect to the spatial variable. For SWCNTs, R_t the radius, w_t the radial displacement, E Young's modulus, h the tube thickness, D the flexural rigidity, ρ_t the mass density per unit area, L the length; For water shell, ρ_f the mass density per unit area, R_f the radius, w_f the radial displacement, γ the CNT–water surface tension, ρ_{water} the mass density per unit bulk of the potential flow, p the radial pressure executed on the water shell due to the water in the center of the SWCNTs, and c is the vdW interaction coefficient which can be obtained via a continuum Lennard-Jones potential [7]

$$U(s) = K\left[\left(\frac{s_0}{s}\right)^4 - 0.4\times\left(\frac{s_0}{s}\right)^{10}\right], \tag{5}$$

where $-0.6K$ is the well depth, s the interlayer spacing between the SWCNTs and the water shell. c is the second derivative of (5) at equilibrium distance s_0, that is expressed as

$$c(s_0) = -\frac{24K}{s_0^2} \tag{6}$$

For simply supported water-filled SWCNTs, the solution of Eqs. (1) and (2) can be obtained by

$$w_t = \sum_{m=1}^{2} A_{m,n}(t)\sin(m\pi x / L)\cos(n\theta), \tag{7}$$

$$w_f = \sum_{m=1}^{2} A_{m+2,n}(t)\sin(m\pi x / L)\cos(n\theta), \tag{8}$$

where $A_{m,n}(t)$ is the unknown function of time. m is the m^{th} axial mode, and n is the n^{th} circumferential mode. Substituting Eqs. (7) and (8) into the right-hand side of Eq. (3), the differential equations for the stress function F are easily yielded.

In fact, on the Galerkin projection principle, a more general orthogonal relationship is written as

$$\int_0^L \int_0^{2\pi} X_i \cdot Z_s(x,\theta) d\theta dx = 0. \tag{9}$$

From Eqs. (1) and (2), letting X_i and Z_s be

$$X_1 = D\nabla^4 w_t + \rho_t \frac{\partial^2 w_t}{\partial t^2} + c\left(w_t - w_f\right) - \frac{1}{R_t}\frac{\partial^2 F}{\partial x^2}, \tag{10}$$

$$X_2 = \gamma\frac{\partial^2 w_f}{\partial x^2} + \frac{R_t}{R_f}c\left(w_t - w_f\right) - p - \rho_f\frac{\partial^2 w_f}{\partial t^2} \tag{11}$$

$$Z_s(x,\theta)=\begin{cases}\cos(n\theta)\sin\left(\dfrac{\pi x}{L}\right), s=1,3\\ \cos(n\theta)\sin\left(\dfrac{2\pi x}{L}\right), s=2,4\end{cases}. \tag{12}$$

Thus, a set of the linear ordinary differential equations for the unknown functions $A_{m,n}(t)$ are obtained as

$$\ddot{A}_{1,n}(t)+\left(\omega_{1n}^2+\frac{c}{\rho_t}\right)A_{1,n}(t)-\frac{c}{\rho_t}A_{3,n}(t)=0 \tag{13}$$

$$\ddot{A}_{2,n}(t)+\left(\omega_{2n}^2+\frac{c}{\rho_t}\right)A_{2,n}(t)-\frac{c}{\rho_t}A_{4,n}(t)=0 \tag{14}$$

$$\begin{aligned}&\ddot{A}_{3,n}(t)+\frac{1}{\rho_f+m_{3n}}\left(\frac{cR_t}{R_f}+\frac{\pi^2\gamma-\pi^2U^2m_{3n}}{L^2}\right)A_{3,n}(t)\\&-\frac{16Um_{4n}}{3L(\rho_f+m_{3n})}\dot{A}_{4,n}(t)-\frac{cR_t}{R_f(\rho_f+m_{3n})}A_{1,n}(t)=0\end{aligned} \tag{15}$$

$$\begin{aligned}&\ddot{A}_{4,n}(t)+\frac{1}{\rho_f+m_{4n}}\left(\frac{cR_t}{R_f}+\frac{4\pi^2\gamma-4\pi^2U^2m_{4n}}{L^2}\right)A_{4,n}(t)\\&+\frac{16Um_{3n}}{3L(\rho_f+m_{4n})}\dot{A}_{3,n}(t)-\frac{cR_t}{R_f(\rho_f+m_{4n})}A_{2,n}(t)=0\end{aligned} \tag{16}$$

Furthermore, Eqs. (13)-(16) are converted into the state space with eight first-order differential equations and the corresponding matrix form is as follows

$$\dot{A}_{1,n}(t)=q_1(t) \tag{17}$$

$$\dot{q}_1(t)=-\left(\omega_{1n}^2+\frac{c}{\rho_t}\right)A_{1,n}(t)+\frac{c}{\rho_t}A_{3,n}(t) \tag{18}$$

$$\dot{A}_{2,n}(t)=q_2(t) \tag{19}$$

$$\dot{q}_2(t)=-\left(\omega_{2n}^2+\frac{c}{\rho_t}\right)A_{2,n}(t)+\frac{c}{\rho_t}A_{4,n}(t) \tag{20}$$

$$\dot{A}_{3,n}(t)=q_3(t) \tag{21}$$

$$\begin{aligned}&\dot{q}_3(t)=-\frac{1}{\rho_f+m_{3n}}\left(\frac{cR_t}{R_f}+\frac{\pi^2\gamma-\pi^2U^2m_{3n}}{L^2}\right)A_{3,n}(t)\\&+\frac{16Um_{4n}}{3L(\rho_f+m_{3n})}\dot{A}_{4,n}(t)+\frac{cR_t}{R_f(\rho_f+m_{3n})}A_{1,n}(t)\end{aligned} \tag{22}$$

$$\dot{A}_{4,n}(t)=q_4(t) \tag{23}$$

$$\dot{q}_4(t) = -\frac{1}{\rho_f + m_{4n}}\left(\frac{cR_t}{R_f} + \frac{4\pi^2\gamma - 4\pi^2U^2 m_{4n}}{L^2}\right)A_{4,n}(t) - \frac{16Um_{3n}}{3L(\rho_f + m_{4n})}\dot{A}_{3,n}(t) + \frac{cR_t}{R_f(\rho_f + m_{4n})}A_{2,n}(t) \tag{24}$$

where

$$\omega_{1n}^2 = \frac{1}{\rho_t}\left(D\left(\frac{\pi^2}{L^2} + \frac{n^2}{R_t^2}\right)^2 + \frac{Eh\pi^4}{R_t^2L^4}\Bigg/\left(\frac{\pi^2}{L^2} + \frac{n^2}{R_t^2}\right)^2\right) \tag{25}$$

$$\omega_{2n}^2 = \frac{1}{\rho_t}\left(D\left(\frac{4\pi^2}{L^2} + \frac{n^2}{R_t^2}\right)^2 + \frac{16Eh\pi^4}{R_t^2L^4}\Bigg/\left(\frac{4\pi^2}{L^2} + \frac{n^2}{R_t^2}\right)^2\right) \tag{26}$$

$$m_{3n} = \frac{\rho_{water}LI_n(\pi R_f/L)}{\pi I_n'(\pi R_f/L)}, \quad m_{4n} = \frac{\rho_{water}LI_n(2\pi R_f/L)}{2\pi I_n'(2\pi R_f/L)} \tag{27}$$

Eqs.(17)-(24) can also be written as a matrix form, [C] is the coefficient matrix, then the characteristic equation of the coupled system is stated as

$$\det(\lambda[I] - [C]) = 0, \tag{28}$$

where [I] is an identity matrix, λ is the eigenvalue of the system. Generally, the eigenvalue is a complex number. Its real part is regarded as a “damping mechanism” resulting from the flow energy transfer from the moving fluid to the SWCNTs and the imaginary part stands for the modal frequency of the system. Obviously, the eigenvalue is a function of the flow velocity.

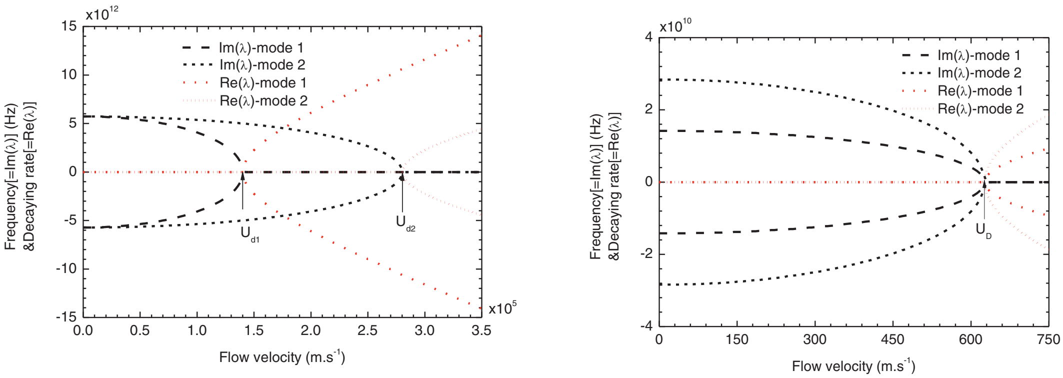
3. Results and discussions

The dynamical simulations are performed on a（20，20）SWCNT at 300 K. The values of material constants are $Eh = 360\text{J/m}^2$, $D = 2eV$, $\rho_t = (2.27\ \text{g/cm}^3) \times 0.34\text{nm}$ [8]. The values of ρ_f, γ, c and s can be extracted by fitting the double shell model to the MD simulations [6].

As examples, the case $n = 5$ with the aspect ratio $L/R_t = 50$ is considered.

Firstly, the dynamic characteristics of the water shell are investigated. Mathematically, the evolution of a system towards divergence or flutter may be tracked by plotting the complex eigenvalues in the plane. So, in this paper, the diagrams for the evolution of the real and imaginary parts of the eigenvalues of the water shell as the flow velocity U are plotted in Fig1. Obviously, the internal moving fluid has a substantial effect on vibration frequencies $(= \mathrm{Im}(\lambda))$ and the decaying rate $(= \mathrm{Re}(\lambda))$ of the water shell. The frequencies decrease as the flow velocity increases until the lowest frequency reduces to zero at a critical flow velocity (U_{di}, or U_{Di}), where a static structural instability-a pitchfork bifurcation divergence appears, after that the system loses stability due to having a positive real part. Meanwhile, it can be seen that the frequencies in Fig.1(a) are larger than those in Fig.1(b) which implied that the existence of vdW interaction improves the natural frequencies of water shell. At last, we can also see that the values of the critical velocities are smartly increased when the vdW interaction is considered which indicates that the critical velocities are affected significantly by the vdW interaction. In other words, the vdW interaction is significant to preserve the stability of the system.

Next, the dynamic behaviors of the SWCNTs are examined. The natural frequencies of SWCNTs with various fluid velocities are listed in Table 1. It can be seen that the variation of natural frequencies is very small, which indicates that fluid velocity has very little influence on the dynamic characteristics of the SWCNTs. In addition, it is observed that the vdW interaction between the SWCNTs and the water shell is responsible for the up-shift of the natural frequencies of SWCNTs which qualitatively accords well with those in Ref.6.



(a) with vdW interaction (b) without vdW interaction

FIG. 1. Evolution of the imaginary and real parts of the eigenvalue with velocity for n =5.

Table 1 Natural frequencies (x10^{10}) of the SWCNTs

Velocity (km/s)	Frequency: With vdW interaction, Mode 1	Frequency: With vdW interaction, Mode 2	Frequency: Without vdW interaction
0	1176.87	1177.11	
3	1176.87	1177.09	
6	1176.85	1177.03	876.16
9	1176.83	1176.93	
12	1176.80	1176.80	

4. Conclusion

The free vibration of water-filled SWCNTs is studied by a double shell-potential flow model in the paper. Results reveal that vdW interaction between the SWCNTs and the water shell is responsible for an upshift in the frequency of the SWCNTs and an improvement in the stability of the system. Furthermore, it is found that the internal moving fluid plays an important role in the instability of system but the flow velocity has very little influence on the dynamic characteristics of the SWCNTs.

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